ECE 371
Materials and Devices

09/26/19 - Lecture 10

Effective Mass, Density of States

General Information

- Homework #3 assigned, due Tuesday 10/1
- Midterms returned by next Thursday
- Midterm solutions posted
- Reading for next time: 3.5, 4.1

Effective Mass Concept

- Movement of an electron in a crystal lattice is different from that in free space
  - Influence of positively charged ions
  - Influence of other electrons

$$F_{total} = F_{ext} + F_{int}$$

- Since we don't know F_{int} very well, we fold it into an "effective mass" (m*)
- Effective mass is given in units of m_0
- Can be higher or lower than m_0
- Can be negative! (hole)
- Allows us to treat electrons in a crystal as classical particles using Newtonian mechanics
- Effective mass influences measurable device properties (current transport in transistors, efficiency of LEDs and solar cells)

temp,

The Parabolic Approximation

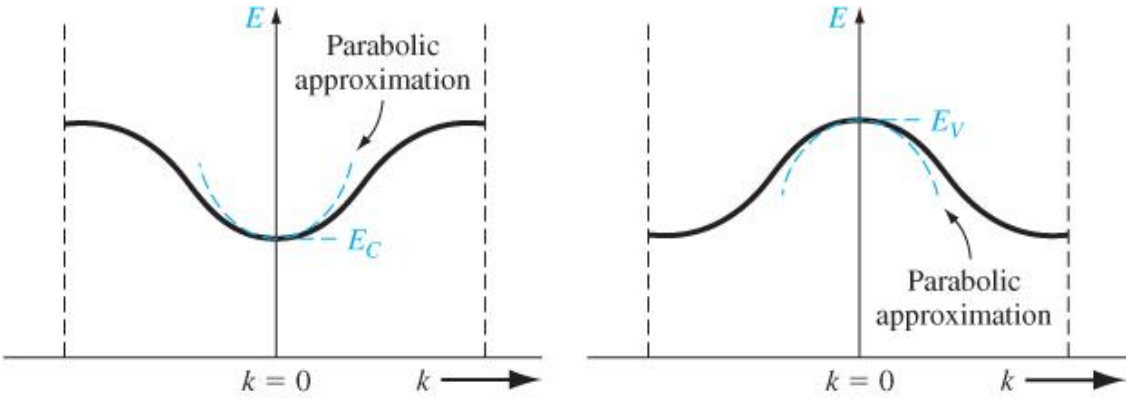


Figure 3.16 | (a) The conduction band in reduced k space, and the parabolic approximation. (b) The valence band in reduced k space, and the parabolic approximation.

- A free electron has a parabolic dispersion curve (E vs. k)
- The dispersion curves for electrons in crystals are roughly parabolic near the bottom (top) of the conduction (valence) bands

Concept of Hole Motion

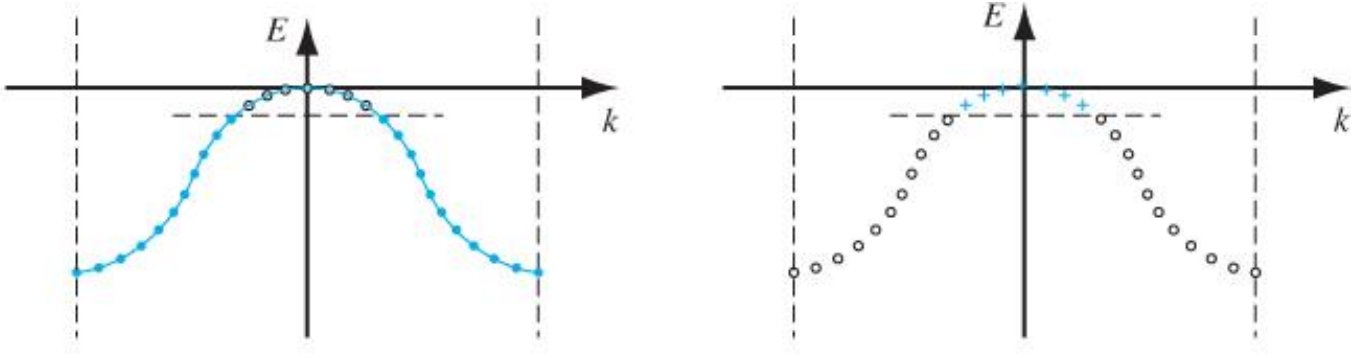


Figure 3.18 | (a) Valence band with conventional electron-filled states and empty states. (b) Concept of positive charges occupying the original empty states.

Empty electron states → Positive charges occupying empty states

*see in-class derivation

Downward parabola starting @ E_V ↑ valence

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{dE}{dk^2} = \frac{-2C_2}{\hbar^2} \rightarrow$$ C_2 is positive, m^* is negative

* electron moving near the top of a band has negative effective mass

(instead of using negative, use a positive effectiveness → hole m_p^*

More on Effective Mass

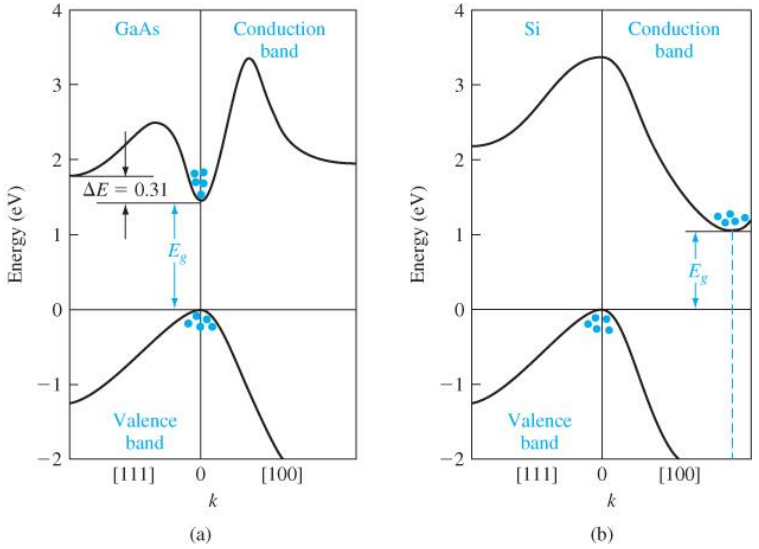


Figure 3.25 | Energy-band structures of (a) GaAs and (b) Si. *(From Sze [12].)*

$$m^* = \frac{\hbar^2}{d^2E / dk^2}$$

Density of states effective mass

Material	m_n^*/m_0	m_p^*/m_0
Si	1.08	0.56
GaAs	0.067	0.48
GaN	0.2	1.2

- m* depends upon energy (k) and direction of electron movement in the crystal
- Also, there are several different effective masses in the valence band (heavy hole (HH), light hole (LH), split-off (SO))
- *Use "density of state effective mass" in this class (see Appendix F and Table B4)*
- *Density of states effective mass is an "average" effective mass over all directions*

Test Your Understanding

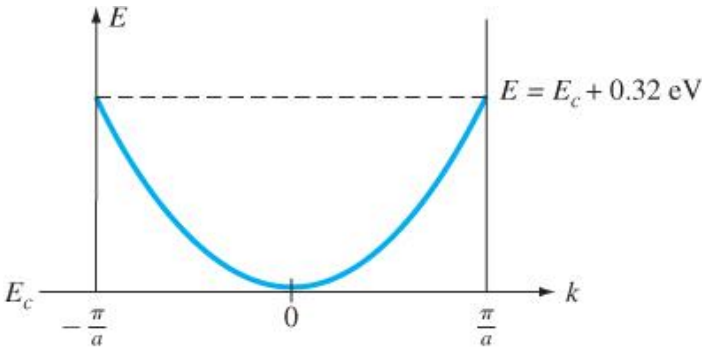


Figure 3.22 | Figure for Exercise TYU 3.3.

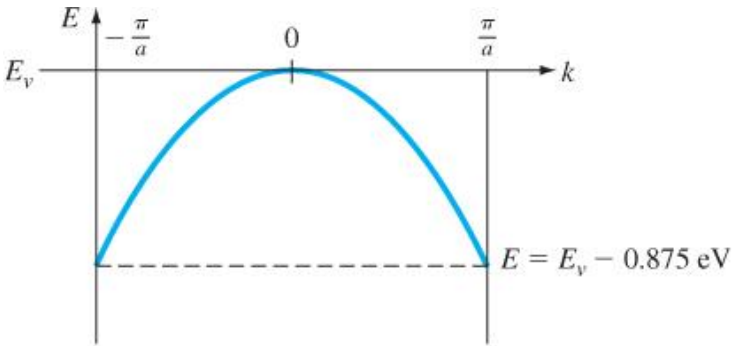


Figure 3.23 | Figure for Exercise TYU 3.4.

TYU 3.3 A simplified E versus k curve for an electron in the conduction band is given. The value of a is 10 Å. Determine the relative effective mass m^*/m_0.
(Ans. $m^*/m_0 = 1.175$)

TYU 3.4 A simplified E versus k curve for a hole in the valence band is given. Assume a value of $a = 12$ Å. Determine the relative effective mass $|m^*/m_0|$.
(Ans. $|m^*/m_0| = 0.2985$)

TYU 3.3 | remember: $m^* = \dfrac{\hbar^2}{\dfrac{d^2E}{dk^2}}$

need $E(k) = Ck^2 + E_c$ if dealing with valence instead, $E(k) = E_v - Ck^2$

$$E\left(\frac{\pi}{a}\right) = C\left(\frac{\pi}{a}\right)^2 + \cancel{E_c} = \cancel{E_c} + 0.32\,eV$$

$$C = (0.32\,eV)\frac{a^2}{\pi^2}$$

$$\frac{d^2E}{dk^2} = 2C = 2(0.32\,eV)\frac{a^2}{\pi^2}$$

$$m^* = \frac{\hbar^2}{2(0.32\,eV)\dfrac{a^2}{\pi^2}}$$

a is given
$10\,\text{Å} = 10^{-10}\,m$

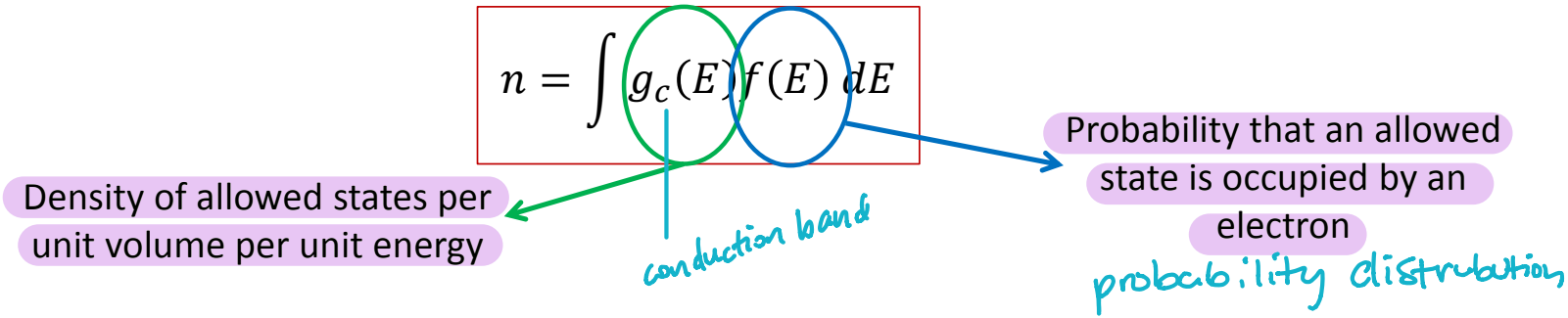
$$= 1.07 \times 10^{-30}\,kg$$

$$m_o = \frac{m^*}{9.11 \times 10^{-31}} = 1.175$$

written as $1.175\,m_o$

Carrier Density and Density of States

- Goal: determine the electron (n) and hole (p) densities (#/cm^3) in the semiconductor



- The density of states (DOS) describes the density of allowed states per unit volume per unit energy (g(E))
- Electron and holes are called "carriers"
- First we will calculate the DOS portion of the carrier density

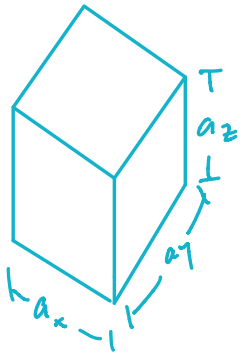
Electron density

$$n = \int g_c(E) f(E)\, dE$$

$g_c(E)$: density $\left(\frac{\#}{\text{energy} \cdot \text{vol}}\right)$

$f(E)$: probability that an allowed state is occupied by electron

count up the # of K states



$V(x,y,z) = 0$ inside

$V(x,y,z) = \infty$ outside

(infinite potent. box)

$$\psi(x,y,z) = A \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right) \sin\left(\frac{n_z \pi}{a} z\right)$$

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} \left(n_x^2 + n_y^2 + n_z^2\right)$$

(1 1 1) is the lowest possible ground state in 3D

$$k_x = \frac{n_x \pi}{a}, \quad k_y = \frac{n_y \pi}{a}, \quad k_z = \frac{n_z \pi}{a}$$

$$k^2 = \frac{\pi}{a}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$\downarrow$$

$$\frac{2mE}{\hbar^2}$$

What is the area of one state?

$$k_{x+1} - k_x \rightarrow (n_x + 1)\frac{\pi}{a} - n_x \frac{\pi}{a} = \frac{\pi}{a}$$

separation between states

Then area is $\left(\frac{\pi}{a}\right)^2$

Volume of single state in k-space

$$V_k = \left(\frac{\pi}{a}\right)^3$$

Then D.O.S. $\rightarrow$ $g(E) = \frac{1}{V}\frac{dN_s}{dE}$

N_s: # states; E: energy; V: volume (a^3)

$$\left[\frac{\#\text{ states}}{\text{vol} \cdot \text{energy}}\right]$$

Density of States (DOS)

- To determine the 3D DOS in k-space:

1. Calculate the number of states ($N_s(k)$) as a function of k contained within the sphere bounded by $k^2 = k_x^2 + k_y^2 + k_z^2$ by taking the volume of the sphere in k-space ($V_{sphere} = (4/3)\pi k^3$) divided by unit volume of one state in k-space ($V_{unit-k} = (\pi/a)^3$)
2. Multiply by 2 for spin degeneracy and divide by 8 to keep only positive k-values
3. Using the parabolic approximation for a free electron, convert $N_s(k)$ to $N_s(E)$
4. Divide by a unit volume in real space $V_{unit} = a^3$
5. Differentiate with respect to E, dN_s/E, to get the DOS

gives constant energy surface

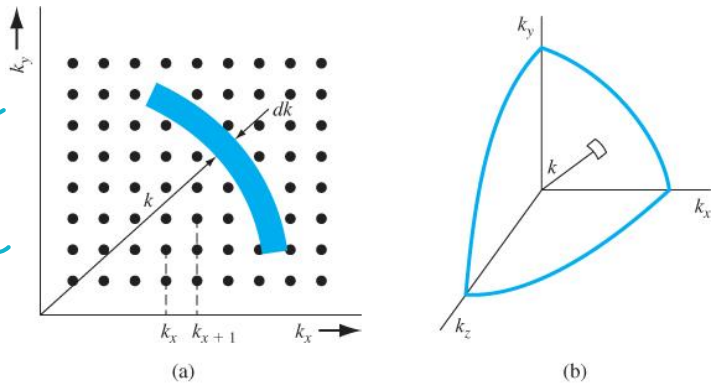


Figure 3.26 | (a) A two-dimensional array of allowed quantum states in k space. (b) The positive one-eighth of the spherical k space.

$$DOS = \frac{1}{V_{unit}} \frac{dN_s}{dE}$$

V_{unit} = unit volume
N_s = # of states
E = energy

(1) $$\frac{V_{sphere}}{V_k} = \frac{\frac{4}{3}\pi k^3}{(\pi/a)^3}$$

(2) # states in $\frac{1}{8}$ sphere: $$N_s(k) = \frac{a^3 k^3}{3\pi^2}$$

(3) $$N_s(E) = \frac{a^3 (2mE)^{3/2}}{3\pi^2 \hbar^3}$$

(4) $$\frac{N_s(E)}{V} = \frac{(2mE)^{3/2}}{3\pi^2 \hbar^3}$$

(5) $$g(E) = \frac{1}{V}\frac{dN_s}{dE}$$

$$= \frac{4\pi (2m)^{3/2}}{h^3}\sqrt{E}$$

Density is proportional to $\sqrt{E}$

Increase energy → increase states, but only to a certain point

Translating

$E \rightarrow E - E_c$ for conduction

$E_v - E$ for valence

$m \rightarrow m_n^*$ for conduction

m_p^* for valence

no states in bandgap

holes typically larger eff. mass than electrons

Semiconductor Density of States (3D)

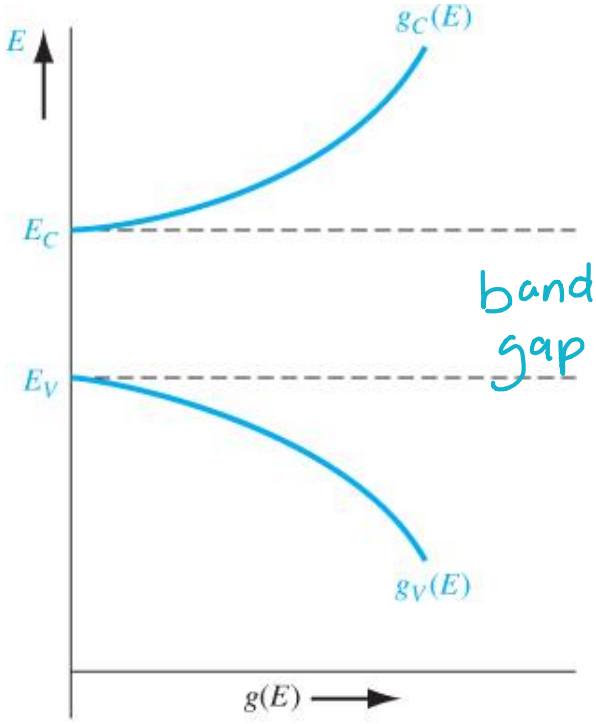


Figure 3.27 | The density of energy states in the conduction band and the density of energy states in the valence band as a function of energy.

Conduction band DOS:

$$g_c(E) = \frac{4\pi}{h^3}[2m_n^*]^{3/2}(E - E_c)^{1/2}$$

Valence band DOS:

$$g_v(E) = \frac{4\pi}{h^3}[2m_p^*]^{3/2}(E_v - E)^{1/2}$$

change E & m to m*

- Parabolic approximation
- Fewer states at lower energies
- No states in the forbidden gap
- In general, $g_c(E)$ and $g_v(E)$ are different
- 3D DOS is also called "bulk" DOS

Density of States (Lower Dimensions)

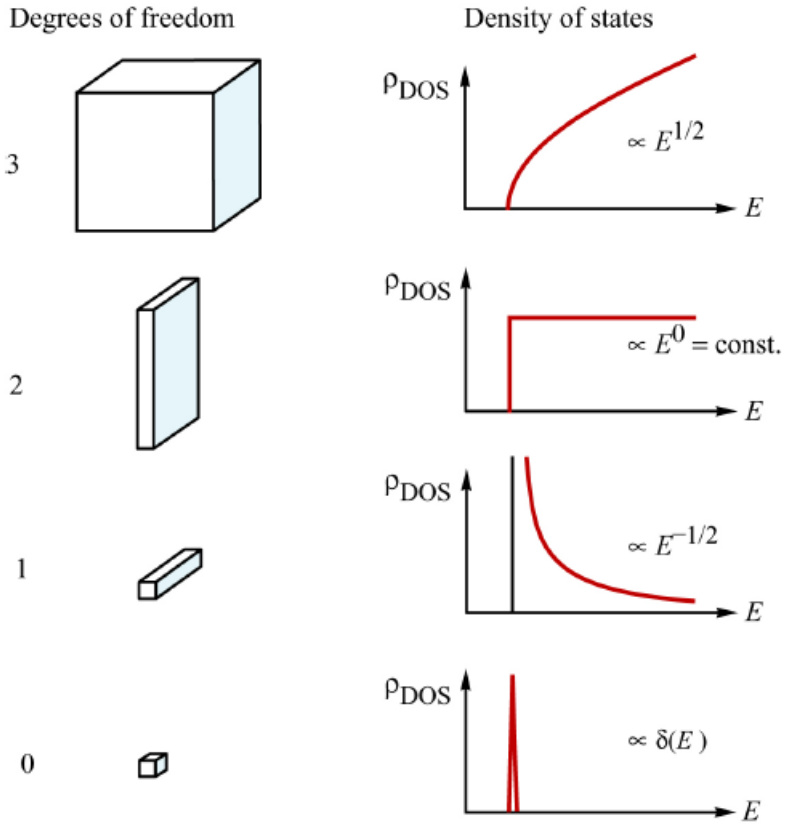


Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

Quantum Well Density of States

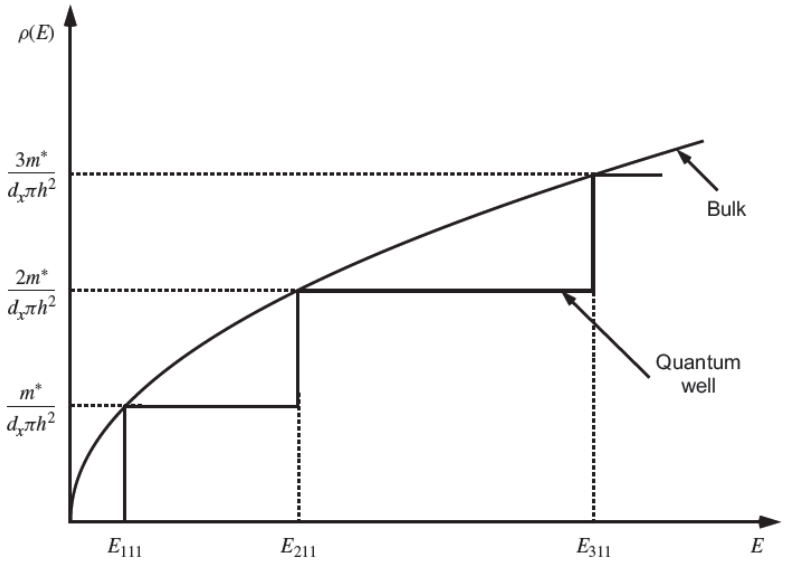


FIGURE A1.13: Density of states for an infinite-barrier quantum well and bulk material. If the barrier is not infinite, the quantum-well energies decrease slightly. If desired, the density of state plateaus can be decreased by using an effective $d_x = d_x^*$ (a different one for each state) so that the extrema continue to intersect the bulk characteristic.

QW DOS:

$$g(E) = \frac{1}{d_x}\sum_{n_x}\frac{m^*}{\pi\hbar^2}\mathcal{H}(E - E_{n_x})$$